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FILE 'HOME' ENTERED AT 09:52:02 ON 18 OCT 2005

=> fil reg
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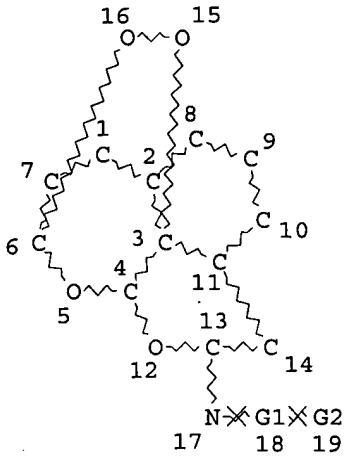

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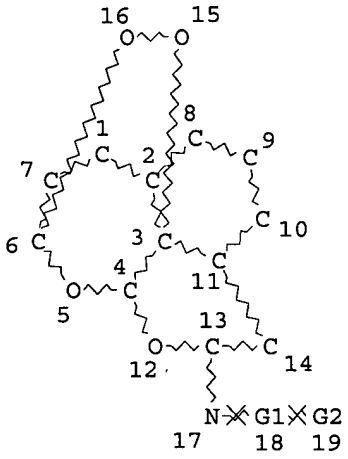

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

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100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

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FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             3 TO      163
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1

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SEARCH TIME: 00.00.01

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2         RN              600141-79-5  REGISTRY
3         RN              390800-28-9  REGISTRY
4         RN              390800-27-8  REGISTRY
5         RN              390800-26-7  REGISTRY
6         RN              390800-25-6  REGISTRY
7         RN              390800-24-5  REGISTRY
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14        RN              128050-94-2  REGISTRY
15        RN              127971-95-3  REGISTRY
16        RN              127971-94-2  REGISTRY
17        RN              127971-93-1  REGISTRY
18        RN              127971-92-0  REGISTRY


=> fil caplus
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=> s l3
L4            8 L3
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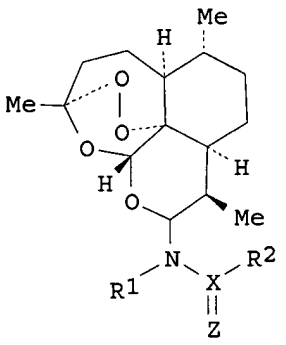
L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

2003:737764 Document No. 139:261439 Preparation of antiparasitic artemisinin derivatives (sesquiterpene endoperoxides). Haynes, Richard K. (Bayer Aktiengesellschaft, Germany; Bayer Business Services GmbH). PCT Int. Appl. WO 2003076446 A1 20030918, 28 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-EP1839 20030224. PRIORITY: EP 2002-5233 20020308.

GI



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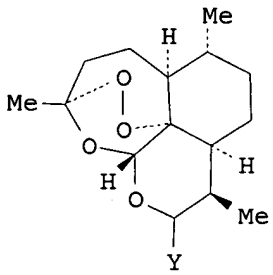


II

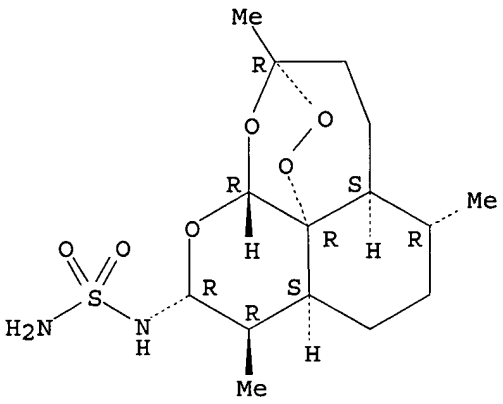
AB This invention relates to certain novel C-10 substituted derivs., e.g., I [R1 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl; R2 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, N(R6)2, NHNH2, NR6NHR6, NR6N(R6)2, OR6, SR6; X = S, S(:O), PR3, P(:O)R3, P(:NR4)R3; R3, R4 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl; Z = O, S, NR5; R5 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl; R6 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, 10α-dihydroartemisinyl, etc.], or a salt, solvate or solvate salt, of artemisinin, a process for their preparation, their use in the treatment and/or prophylaxis of diseases caused by infection with a parasite and pharmaceutical compns. containing such C-10 substituted derivs. A process for the preparation of I comprises reacting dihydroartemisinin derivative II [Y = OH, OSiMe3] with a halogenating agent to give II [Y = halogen]; and, if desired, reacting the latter with an amine, R1NHX(:Z)R2. Thus, 10α-(sulfamino)dihydroartemisinin [I; NR1X(:Z)R2 = NHSO2NH2-α] was prepared from 10α-[(trimethylsilyl)oxy]dihydroartemisinin [II; Y = OSiMe3-α] via reaction with sulfamide in THF.

IT **600141-79-5P 600141-80-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiparasitic artemisinin derivs. (sesquiterpene endoperoxides))

RN 600141-79-5 CAPLUS

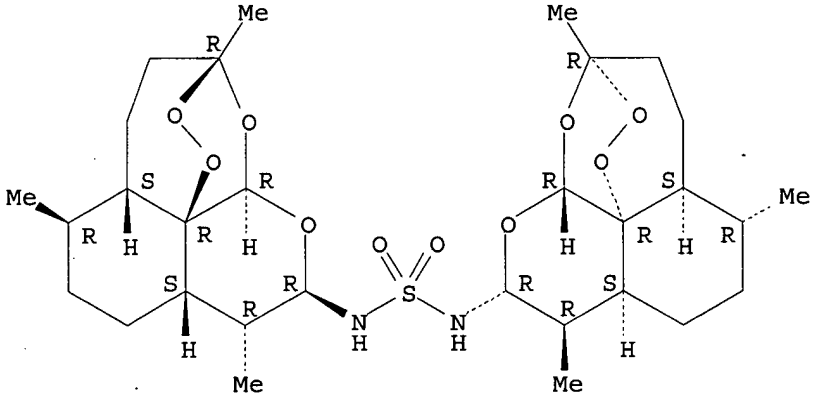
CN Sulfamide, [(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 600141-80-8 CAPLUS
CN Sulfamide, N,N'-bis[(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
2002:105791 Document No. 136:118602 Preparation of arteannuin derivatives containing azacyclic radical. Li, Ying; Liao, Xibin (Shanghai Inst. of Pharmaceutics, Chinese Academy of Sciences, Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 1296009 A 20010523, 15 pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 1999-124012 19991112.
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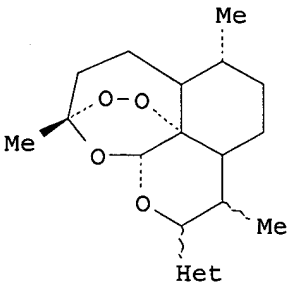

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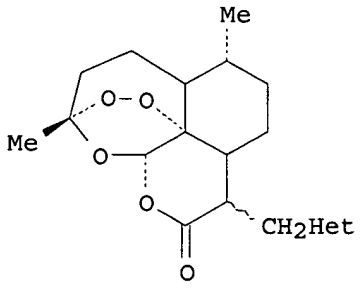
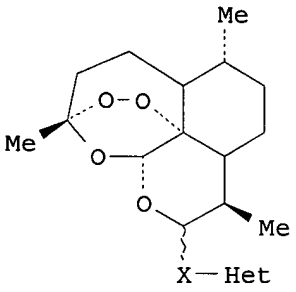


II



III

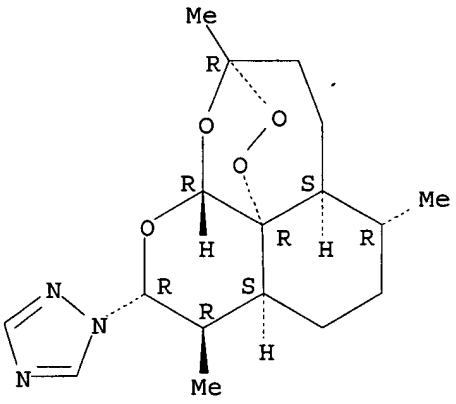
AB Compds. I, II, III (Het = triazole, benzotriazole, benzimidazole, indole, or their derivs. substituted by carboxyl, ester group, acyl, alkoxy, C1-3 alkyl, hydroxy, or hydroxymethyl; X = -OCO-, -OCH2-, -OCH2CH2-, -OCH2CH(OH)CH2-) are claimed. Title compound were synthesized by the condensation of either acetyldihydroarteannuin or (trichloroacetyl)dihydroarteannuin or methylenearteannuin or dihydroarteannuin or arteannuin 2-bromoethyl ether or arteannuin 2,3-epoxypropyl ether with nitrogen heterocyclic compound in the presence of acidic catalyst or alkaline compds or DCC, giving product with 12% to 61% yield. Thus, dihydroarteannuin dissolved in methylenechloride, adding trifluoroacetic acid anhydrate, reacted under 0-5°, forming dihydroarteannuin trifluoroacetate, adding 1,2,4-triazole, using the TLC follow the reaction, after the workup, giving the triazole substituted dihydroarteannuin, with yield 12-20%. Title compds. are of antimalarial, antitumor, immunoregulatory, and anti-inflammatory activity.

IT **390800-25-6P 390800-26-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of arteannuin derivative containing azacyclic group)

RN 390800-25-6 CAPLUS

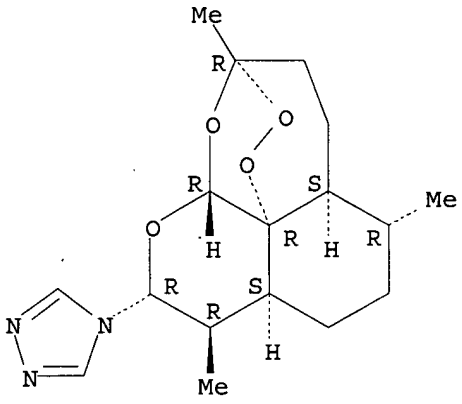
CN 1H-1,2,4-Triazole, 1-[(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



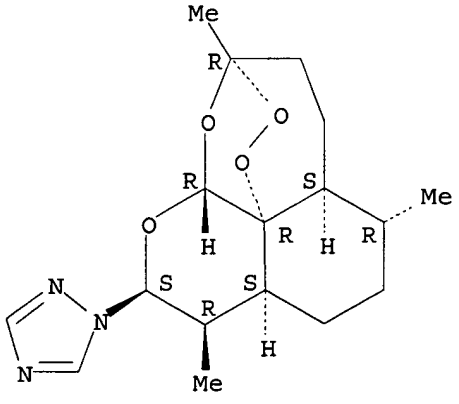
RN 390800-26-7 CAPLUS
CN 4H-1,2,4-Triazole, 4-[(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



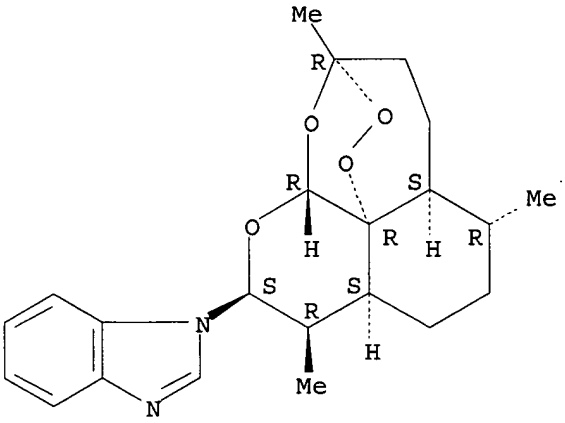
IT **390800-24-5P 390800-27-8P 390800-28-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of arteannuin derivative containing azacyclic group)
RN 390800-24-5 CAPLUS
CN 1H-1,2,4-Triazole, 1-[(3R,5aS,6R,8aS,9R,10S,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



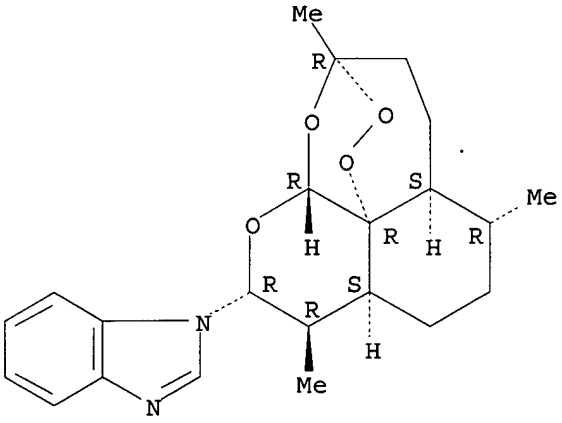
RN 390800-27-8 CAPLUS
CN 1H-Benzimidazole, 1-[(3R,5aS,6R,8aS,9R,10S,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 390800-28-9 CAPLUS
CN 1H-Benzimidazole, 1-[(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



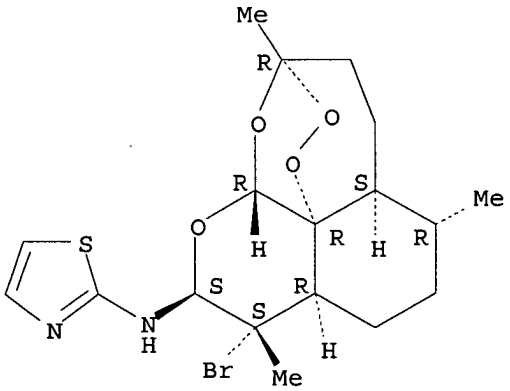
L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
2001:886935 Document No. 136:160854 Structure-Activity Relationships of the Antimalarial Agent Artemisinin. 6. The Development of Predictive In Vitro Potency Models Using CoMFA and HQSAR Methodologies. Avery, Mitchell A.; Alvim-Gaston, Maria; Rodrigues, Carlos R.; Barreiro, Eliezer J.; Cohen, Fred E.; Sabnis, Yogesh A.; Woolfrey, John R. (Department of Medicinal Chemistry School of Pharmacy Thad Cochran National Center for Natural Products Research, University of Mississippi, Mississippi, MS, 38677, USA). Journal of Medicinal Chemistry, 45(2), 292-303 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.
AB Artemisinin (1) is a unique sesquiterpene peroxide occurring as a constituent of Artemisia annua L. Because of the effectiveness of Artemisinin in the treatment of drug-resistant Plasmodium falciparum and its rapid clearance of cerebral malaria, development of clin. useful semisynthetic drugs for severe and complicated malaria (artemether,

artesunate) was prompt. However, recent reports of fatal neurotoxicity in animals with dihydroartemisinin derivs. such as artemether have spawned a renewed effort to develop nontoxic analogs of artemisinin. In our effort to develop more potent, less neurotoxic agents for the oral treatment of drug-resistant malaria, we utilized comparative mol. field anal. (CoMFA) and hologram QSAR (HQSAR), beginning with a series of 211 artemisinin analogs with known in vitro antimalarial activity. CoMFA models were based on two conformational hypotheses: (a) that the x-ray structure of artemisinin represents the bioactive shape of the mol. or (b) that the hemin-docked conformation is the bioactive form of the drug. In addition, we examined the effect of inclusion or exclusion of racemates in the partial least squares (pls) anal. Databases derived from the original 211 were split into chiral (n = 157), achiral (n = 34), and mixed databases (n = 191) after leaving out a test set of 20 compds. HQSAR and CoMFA models were compared in terms of their potential to generate robust QSAR models. The r2 and q2 (cross-validated r2) were used to assess the statistical quality of our models. Another statistical parameter, the ratio of the standard error to the activity range (s/AR), was also generated. CoMFA and HQSAR models were developed having statistically excellent properties, which also possessed good predictive ability for test set compds. The best model was obtained when racemates were excluded from QSAR anal. Thus, CoMFA of the n = 157 database gave excellent predictions with outstanding statistical properties. HQSAR did an outstanding job in statistical anal. and also handled predictions well.

IT **127971-92-0 127971-93-1 127971-94-2**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(QSAR of antimalarial agent artemisinin and development of predictive in vitro potency models using CoMFA and HQSAR)

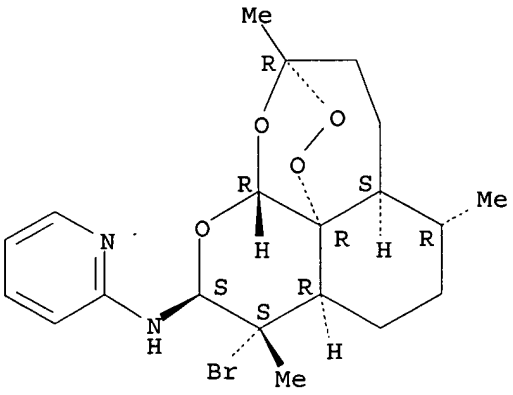
RN 127971-92-0 CAPLUS
CN 2-Thiazolamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



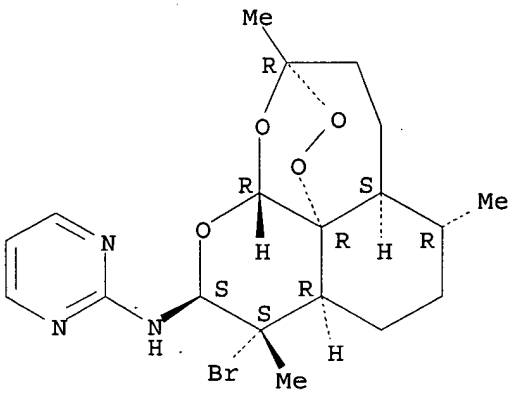
RN 127971-93-1 CAPLUS
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127971-94-2 CAPLUS
CN 2-Pyrimidinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



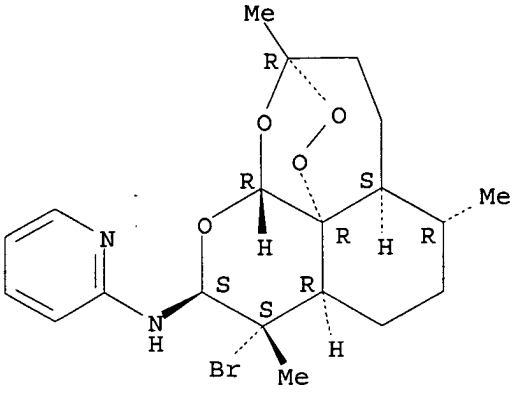
L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
2001:34757 Document No. 134:231512 QSAR study of antimalarial activities and artemisinin-heme binding properties obtained from docking calculations. Tonmunphean, Somsak; Parasuk, Vudhichai; Kokpol, Sirirat (Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand). Quantitative Structure-Activity Relationships, 19(5), 475-485 (English) 2000. CODEN: QSARDI. ISSN: 0931-8771. Publisher: Wiley-VCH Verlag GmbH.

AB The quant. structure-activity relationships (QSAR) between antimalarial activities and artemisinin-heme binding properties were studied by means of docking calcns. Automated mol. dockings of 30 artemisinin derivs. to heme revealed a significant relationship between biol. activity and binding energy (r = -0.93) and less significantly with the O1-Fe distance (r = -0.55). The QSAR models were constructed and the predicted biol. activities were in good agreement with the corresponding exptl. values. The docking also showed that artemisinin compds. approach heme by pointing O1 at the endoperoxide linkage toward the iron center, a mechanism controlled by the steric hindrance.

IT **127971-93-1 127971-94-2 330658-43-0**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(QSAR study of antimalarial activities and artemisinin-heme binding properties obtained from docking calcns.)

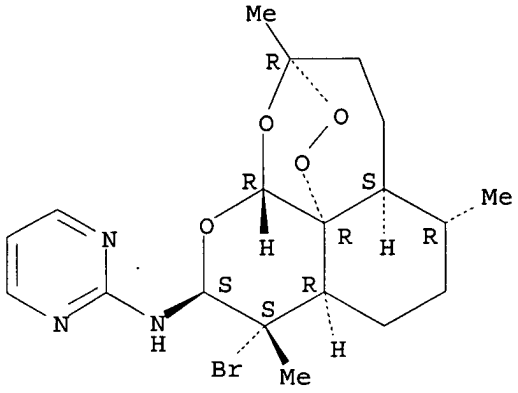
RN 127971-93-1 CAPLUS
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



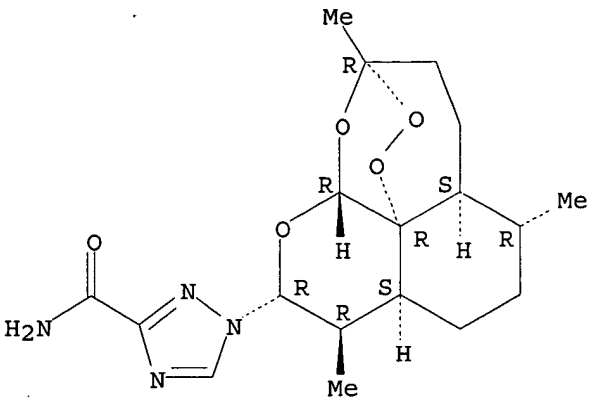
RN 127971-94-2 CAPLUS
CN 2-Pyrimidinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 330658-43-0 CAPLUS
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aS,9R,10S,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

1998:663601 Document No. 130:32682 Comparative molecular field analysis of artemisinin derivatives: ab initio versus semiempirical optimized structures. Tonmunphean, Somsak; Kokpol, Sirirat; Parasuk, Vudhichai; Wolschann, Peter; Winger, Rudolf H.; Liedl, Klaus R.; Rode, Bernd M. (Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand). Journal of Computer-Aided Molecular Design, 12(4), 397-409 (English) 1998. CODEN: JCADEQ. ISSN: 0920-654X. Publisher: Kluwer Academic Publishers.

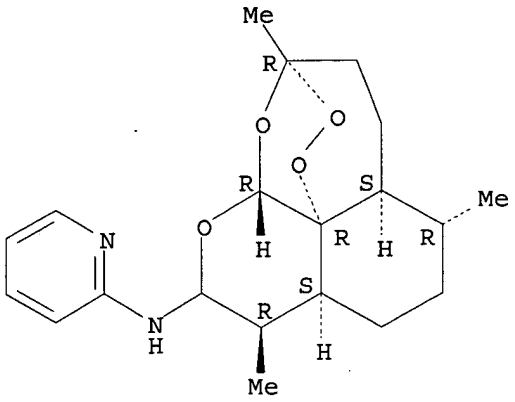
AB Based on the belief that structural optimization methods, producing structures more closely to the exptl. ones, should give better, i.e. more relevant, steric fields and hence more predictive CoMFA models, comparative mol. field analyses of artemisinin derivative antimalarial drugs were performed based on semiempirical AM1 and HF/3-21G optimized geometries. Using these optimized geometries, the CoMFA results derived from the HF/3-21G method are usually but not drastically better than those from AM1. Addnl. calcns. were performed to investigate the electrostatic field difference using the Gasteiger and Marsili charges, the electrostatic potential fit charges at the AM1 level, and the natural population anal. charges at the HF/3-21G level of theory. For the HF/3-21G optimized structures, no difference in predictability was observed, whereas for AM1 optimized structures, such differences were found. Interestingly, if ionic compds. are omitted, differences between the various HF/3-21G optimized structure models using these electrostatic fields were found.

IT **216963-51-8 216963-52-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparative mol. field anal. of artemisinin derivs. using ab initio vs. semiempirical optimized structures)

RN 216963-51-8 CAPLUS

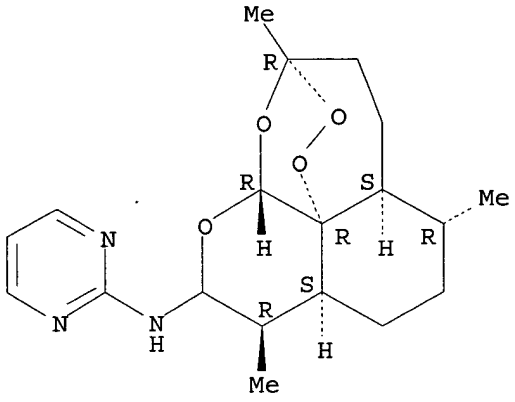
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aS,9R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



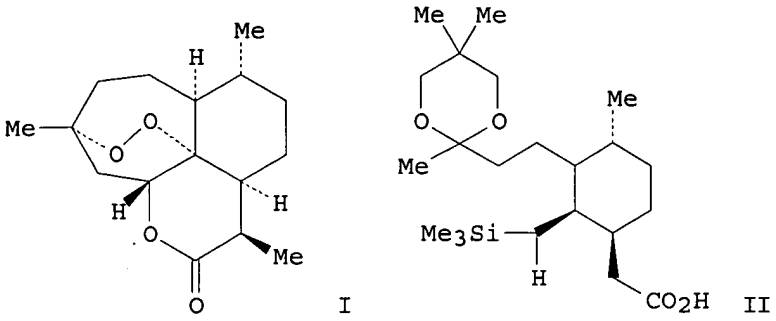
RN 216963-52-9 CAPLUS
CN 2-Pyrimidinamine, N-[(3R,5aS,6R,8aS,9R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



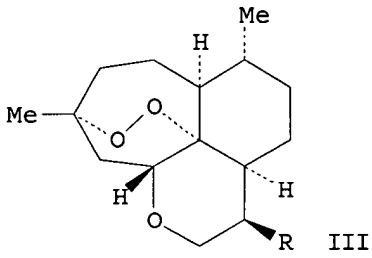
112

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
1994:323882 Document No. 120:323882 Structure-activity relationships of the antimalarial agent artemisinin. 1. Synthesis and comparative molecular field analysis of C-9 analogs of artemisinin and 10-deoxoartemisinin. Avery, Mitchell A.; Gao, Fenglan; Chong, Wesley K. M.; Mehrotra, Sanjiv; Milhous, Wilbur K. (Dep. Chem., Univ. North Dakota, Grand Forks, ND, 58202, USA). Journal of Medicinal Chemistry, 36(26), 4264-75 (English) 1993. CODEN: JMCMAR. ISSN: 0022-2623.
GI



I

II



III

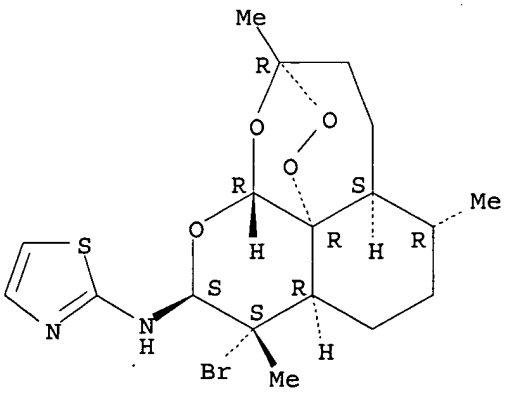
AB A series of C-9 β-substituted artemisinin (I) analogs were synthesized via dianion alkylation of the total synthetic intermediate II followed by subsequent ozonolysis-acidification, or by alkylation of the enolate derived from (+)-9-desmethylartemisinin. 10-Deoxo-9-alkyl derivs. III (R = H, Et) were synthesized convergently from intermediates in the preparation of 9-alkyl derivs. In vitro bioassay was conducted in W-2 and D-6 clones of drug resistant Plasmodium falciparum. Comparative mol. field anal. (CoMFA) of the 9-alkyl lactone derivs. provide a model with a cross-validated r2 = 0.793. Inclusion of inactive 1-deoxyartemisinin analogs IV (R = H, Me, R1 = H, alkyl, allyl) provided a model with a value of 0.857. The activities of a number of other analogs of divergent structure were predicted with good accuracy using the CoMFA model.

IT **127971-92-0 127971-93-1 127971-94-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(predicted relative antimalarial potency of)

RN 127971-92-0 CAPLUS

CN 2-Thiazolamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

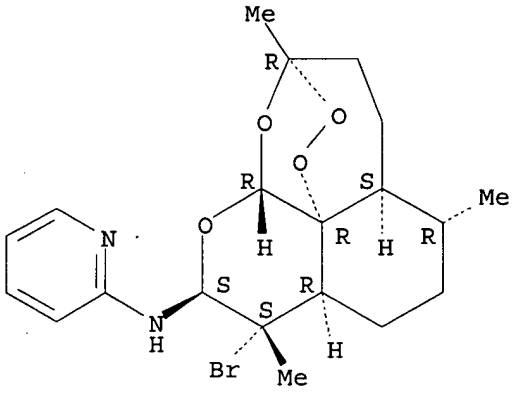
Absolute stereochemistry.



RN 127971-93-1 CAPLUS

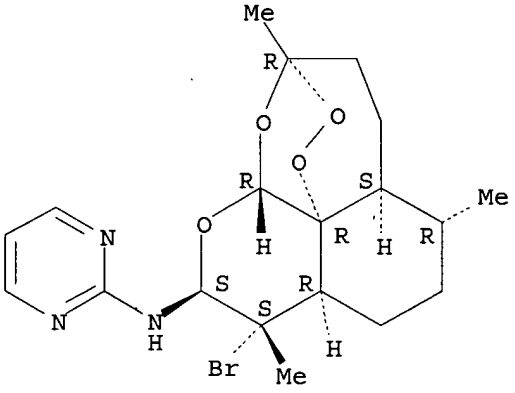
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

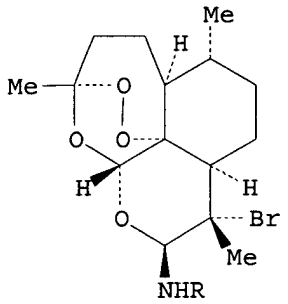


RN 127971-94-2 CAPLUS
CN 2-Pyrimidinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

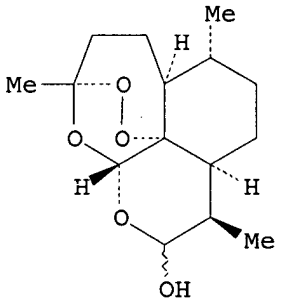
Absolute stereochemistry.



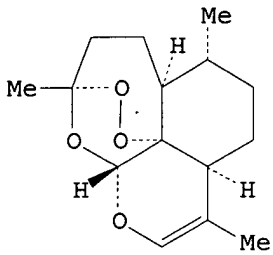
L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
1990:515604 Document No. 113:115604 Antimalarial activity of new water-soluble dihydroartemisinin derivatives. 3. Aromatic amine analogs. Lin, Ai J.; Li, Liang Quan; Klayman, Daniel L.; George, Clifford F.; Flippen-Anderson, Judith L. (Div. Exp. Ther., Walter Reed Army Inst. Res., Washington, DC, 20307-5100, USA). Journal of Medicinal Chemistry, 33(9), 2610-14 (English) 1990. CODEN: JMCMAR. ISSN: 0022-2623. OTHER SOURCES: CASREACT 113:115604.
GI



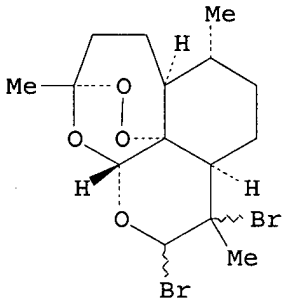
I



II



III



IV

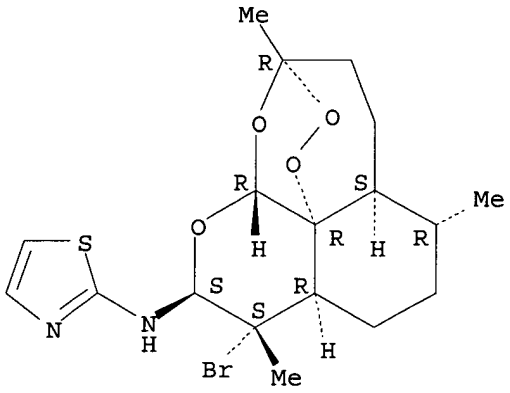
AB A series of artemisinin derivs. I (R = 1,3-thiazol-2-yl, 3-FC6H4, Ph, 2-pyridyl, 2-pyrimidinyl, 5-bromo-2-pyridyl) was prepared in the search for analogs with good water solubility and high antimalarial activity. Treatment of dihydroartemisinin (II) with BF3.OEt2 at room temperature gave the key intermediate, 9,10-dehydrodihydroartemisinin (III), which, on reaction with Br, gave the dibromide IV, which was aminated to give I in 25-55% yield. I, tested in vitro against Plasmodium falciparum, were more effective against W-2 than D-6 clones and were not cross-resistant with existing antimalarials. I (R = 3-FC6H4) was the most active, with the ED50 ≤ 0.16 ng/mL making it several-fold more potent than artemisinin. However, no significant in vivo antimalarial activity against Plasmodium berghei was observed

IT **127971-92-0P 127971-94-2P 127971-95-3P 128050-94-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antimalarial activity of)

RN 127971-92-0 CAPLUS

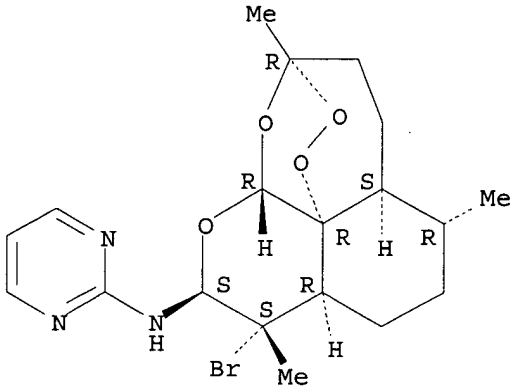
CN 2-Thiazolamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

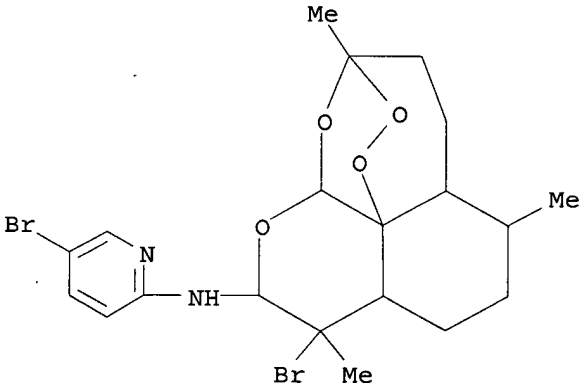


RN 127971-94-2 CAPLUS
CN 2-Pyrimidinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

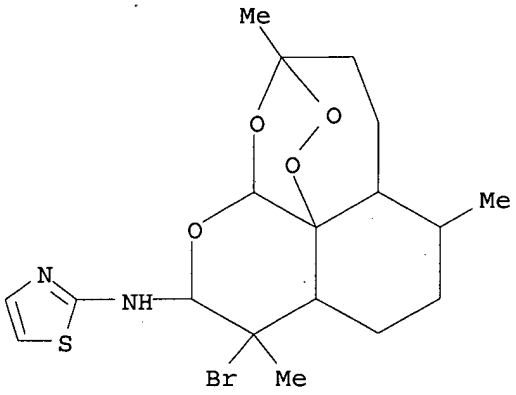


RN 127971-95-3 CAPLUS
CN 2-Pyridinamine, 5-bromo-N-(9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl)-, [3R-(3α,5aβ,6β,8aβ,9β,10α,12β,12aR*)]- (9CI) (CA INDEX NAME)



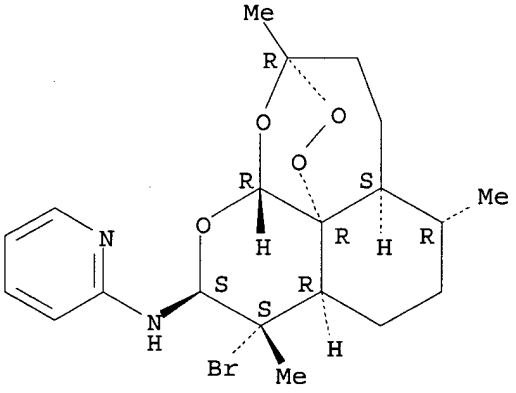
RN 128050-94-2 CAPLUS
CN 2-Thiazolamine, N-(9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl)-, [3R-(3α,5aβ,6β,8a

β,9α,10α,12β,12aR*)]- (9CI) (CA INDEX NAME)



IT **127971-93-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and antimalarial activity of)
RN 127971-93-1 CAPLUS
CN 2-Pyridinamine, N-[(3R,5aS,6R,8aR,9S,10S,12R,12aR)-9-bromodecahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.82	216.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.84	-5.84

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